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Polycrystalline models of anisotropic sintered magnets: Influence of grain alignment on mechanical properties and residual stresses

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ABSTRACT

Models of polycrystalline microstructures, representative for sintered permanent magnets with various grain size distributions and alignment degrees, were generated by the Voronoï tessellation technique. The polycrystalline models were meshed and then a stress/strain analysis was performed with the Finite Element Method (FEM) in order to derive the relation between the homogenized properties (thermal expansion coefficient, elastic constants) and the degree of grain alignment. Residual stresses after sintering were also analyzed and a possible mechanism involved in the decrease in mechanical strength is discussed. It is argued that small sized and poorly aligned grains dispersed in the polycrystalline material are highly stressed after elaboration and could be responsible for the initiation of failure.

1. Introduction

A large amount of dense anisotropic permanent magnets are produced by the powder metallurgy route [1]. The forming process generally involves the compaction of a loose packing of monocrystalline grains that are aligned along a preferential direction, followed by a sintering step. During the powder alignment, each particle rotates in such a way that the easy magnetization axis tends to be parallel to the external magnetic field. As a consequence, polycrystalline anisotropic magnets exhibit highly textured microstructures where each grain has a magnetization close to the saturation level and keeps a low angular misfit with the neighboring grains.

This texturation leads to high performance magnets with optimal energy products. Materials based on the compositions $Nd_2Fe_{14}B$, $(Ba,Sr)Fe_{12}O_{19}$ (hexaferrites) and $SmCo_5/Sm_2Co_{17}$ are the most common anisotropic sintered hard magnets produced at the industrial scale [2]. Each of these crystallographic structures exhibits strong mechanical anisotropy [3,4] that induces detrimental effects during manufacturing. Large geometrical distortions may occur during sintering [5] and high internal thermo-mechanical stresses develop during cooling or subsequent thermal treatments, making the production of net-shape and defect-free magnets more complicated [6]. This is especially the case for annular radially oriented magnet where radial cracks inevitably appear in thick parts during cooling in sintering furnaces [6,7].

Sintered permanent magnets are most often brittle materials and are very sensitive to tensile stresses and mechanical impact. They have to be carefully machined and kept from mechanical loading in the applications. The mechanical robustness depends on many microstructural features, such as the grain size dispersion and morphology [8], the grain alignment degree, the presence of intergranular weak phases and, also, on residual stresses [9]. Fracture generally develops in sintered magnets by an intergranular mode [6,9,10]. For a given microstructure, it has been reported that alignment and grain texturation tend to reduce the mechanical strength of the sintered magnets [11].

The purpose of this paper is to investigate the relation between the mechanical properties of ferromagnetic polycrystalline materials and the grain size distribution and orientation. Voronoï tessellation technique was used to generate models of two and three-dimensional microstructures. Once polycrystalline models with representative grain size distribution were obtained, the crystallographic orientation was attributed to each grain to reproduce the effect of the alignment field on powders. Indeed, it has been reported that alignment field has a better efficiency on large particles compared to the small ones, leading to microstructures with large and well aligned grains surrounded by small randomly oriented grains [12]. The post-sintering residual stresses in these microstructures were analyzed by the Finite Element Method (FEM).

The paper is organized as follows: in Section 2 the

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methodology used to obtain polycrystalline models of sintered magnets is exposed. Section 3 details the thermo-mechanical calculations performed on the polycrystalline microstructures and the results are analyzed in Section 4. In Section 5, a possible mechanism involved in the decrease in the mechanical strength of sintered parts is discussed. It is argued that small sized and poorly aligned grains dispersed in the polycrystal are highly stressed after elaboration. This localization of stresses could be responsible for the initiation of failure and could explain the decrease in the mechanical strength of aligned sintered magnets.

2. Method for the generation of polycrystalline models by Voronoï tessellation

Voronoï tessellation allows two or three-dimensional domains to be partitioned into polygonal or polyhedral cells that completely fill the initial space [13]. The morphological features of these faceted cells are found to be close to the geometrical properties of grain boundaries encountered in real polycrystalline materials [14]. The technique has been widely used to supply representations of polycrystalline microstructures from which numerical simulations can be performed in order to estimate different macroscopic properties. For instance, by performing strain/stress analysis at the grain scale, it has been possible to clarify the role of grains on some mechanical properties (plasticity, damage) for a wide range of materials [15,16]. Trajectories of intergranular cracks in graded and heterogeneous microstructures can also be analyzed [17,18]. For magnetic materials, Voronoï tessellation has been coupled with micro-magnetic models in order to investigate the coercivity of hard magnets [19].

However, special attention should be paid for modeling polycrystals with a broad range of grain size. Moreover, the statistics of cell size achievable by the tessellation method cannot be easily adjusted to actual grain size distribution [20]. The methodology used to account for log-normal size distributions, suited to actual microstructures [21], is detailed in the following sections.

2.1. Classical Voronoï tessellation

The initial step of the method consists in the realization of N points S_i distributed in the domain Ω to be partitioned. Each point will act as a so-called seed and the whole set of seeds will give rise to N cells. Each cell is defined as the sub-domain C_i that contains all points that are closer to the seed S_i than any other seed $S_{j\neq i}$ [20]:

$$C_i = \left\{P \in \Omega | \|PS_i\| < \|PS_{j\neq i}\|\right\} \tag{1}$$

Seeds can be randomly positioned in the domain without any spacing constraint or selected under the condition that a minimal distance δ should be kept between every couple of seeds [14]:

$$\forall\ P_i, P_j \quad \|P_iP_j\| > \delta \tag{2}$$

It is convenient to introduce a typical distance D_{reg} for normalization purpose. In a 2D partition, this distance corresponds to the size of N identical hexagonal cells that cover the domain of area A. If S denotes the cell area ($S=A/N$), it comes

$$D_{reg} = \sqrt{\frac{2S}{\sqrt{3}}} = \sqrt{\frac{2A}{N\sqrt{3}}} \tag{3}$$

For a 3D domain of volume V, the distance corresponds to the size of a tetrakaidecahedron solid:

$$D_{reg} = \sqrt[3]{\frac{3V\sqrt{3}}{8N\sqrt{2}}} \tag{4}$$

A parameter denoted α is defined to evaluate the regularity of the Voronoï partition:

$$\alpha = \frac{\delta}{D_{reg}} \tag{5}$$

A value of α equal to 1 corresponds to a partition made of regular solids while for $\alpha = 0$ the cells tend to be more randomly sized [14]. The minimal allowable distance between two seeds, δ, becomes a control parameter of the cell size distribution in the classical Voronoï tessellation. Zhang et al. [14] found that the standard deviation of the cell size distribution tends to rise from 0 ($\alpha=1$) to a maximal value when $\alpha=0$. Using a log-normal distribution to analyze the cell length distribution (see Appendix A), we found in this work a maximal value for the geometric standard deviation (denoted standard deviation hereafter) of cell length that is equal to 0.27 for $\alpha=0$ ($N=5000$). This upper bound for the standard deviation is in good agreement with the value given by Tanemura (0.243) related to the distribution of cell perimeters [22]. However, Luther et al. [17] studied real sintered polycrystals characterized by a standard deviation higher than this bound ($\sigma_d > 0.9$) and showed that this microstructure is poorly described by the classical tessellation method.

2.2. Weighted Voronoï tessellation

For the generation of broader cell size distribution the weighted Voronoï tessellation, often called Laguerre tessellation, has revealed to be more efficient [20,23]. Basically, this method consists of associating a distance, or a weight w_j, to each seed S_i in order to construct N cells according to the following rule:

$$C_i = \left\{P \in \Omega | \sqrt{\|PS_i\|^2 - w_i^2} < \sqrt{\|PS_{j\neq i}\|^2 - w_{j\neq i}^2}\right\} \tag{6}$$

Weights can be seen as radii of circles (or spheres in 3D) centered on the corresponding seeds and giving rise to a packing of circular particles that fill the domain. The polyhedral cells obtained with rule Eq. (6) will be sized according to these particles. Thus, the cell size distribution in the partition is closely related to the size distribution of primary circular particles. The most common technique used for positioning the seeds consists in generating a Random Closed Packing (RCP) of disks (or spheres) that leads to a distribution of non-overlapping primary particles [20]. The following condition for the particles centers P_i has to be fulfilled in such a packing:

$$\forall\ P_i, P_j \quad \|P_iP_j\| > w_i + w_j \tag{7}$$

Fan et al. [20] found that broad distributions of cell size can be obtained from RCP. However, this method requires time consuming routine in order to obtain dense packing of particles. In this work, it is proposed to start the partition from a random packing of overlapping particles (disks or spheres) whom centers are distributed in the domain under the spacing constraint that writes:

$$\forall\ P_i, P_j \quad \|P_iP_j\| > \sqrt{w_i^2 + w_j^2} \tag{8}$$

This alternative approach allows a simple and fast algorithm (depicted below) to be used for obtaining broad grain size distributions.

2.3. Procedure for the polycrystalline models generation by weighted tessellation

Two and three dimensional partitions can be performed according to the same procedure. For convenience, only the 2D case is described in the following.